Electronic Supplementary Information (ESI)

Can Ionic Liquids Be Cheap?

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This document reports the details of the methods and results and consists of three main sections. In the first section, experimental details of ILs synthesis are reported. In the second section, details of the simulations and their results are presented for both the conventional and intensified process scenarios. In the third section, the details of the economic analysis and corresponding assumptions are discussed.

1. ILs synthesis

$[HNEt_3][HSO_4]$ (IL1) synthesis: Triethylamine (10.1 g, 0.1 mol) was mixed with 50 ml water and the mixture cooled to 0°C. Sulfuric acid (9.8 g, 0.1 mol) was added drop wise while stirring. The stirring was continued for 1 h at room temperature. ^{1}H-NMR and mass spectra are shown in Figures S1 and S2, respectively.

$[HC_1im][HSO_4]$ (IL2) synthesis: 1-methylimidazole (8.2 g, 0.1 mol) was mixed with 50 ml water and the mixture cooled to 0°C. Sulfuric acid (9.8 g, 0.1 mol) was added drop wise while stirring. The stirring was continued for 1 h at room temperature. ^{1}H-NMR and mass spectra are shown in Figures S3 and S4, respectively.

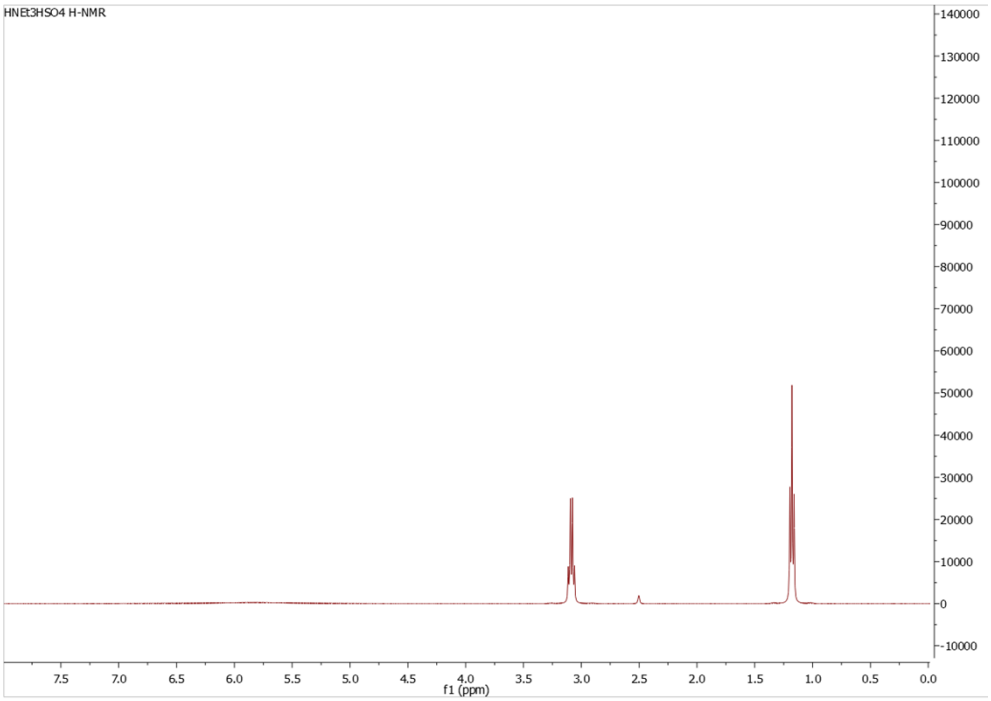


Figure S1 ^{1}H-NMR of IL1

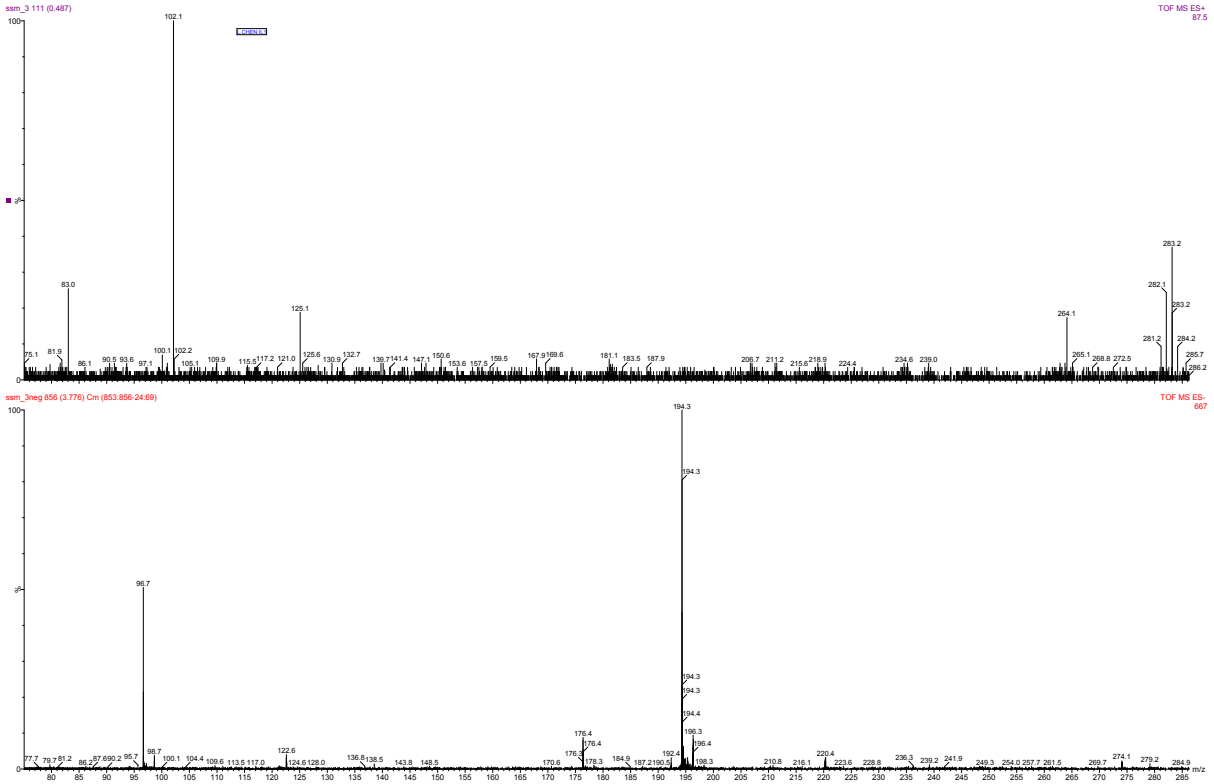


Figure S2 Mass spectra of IL1

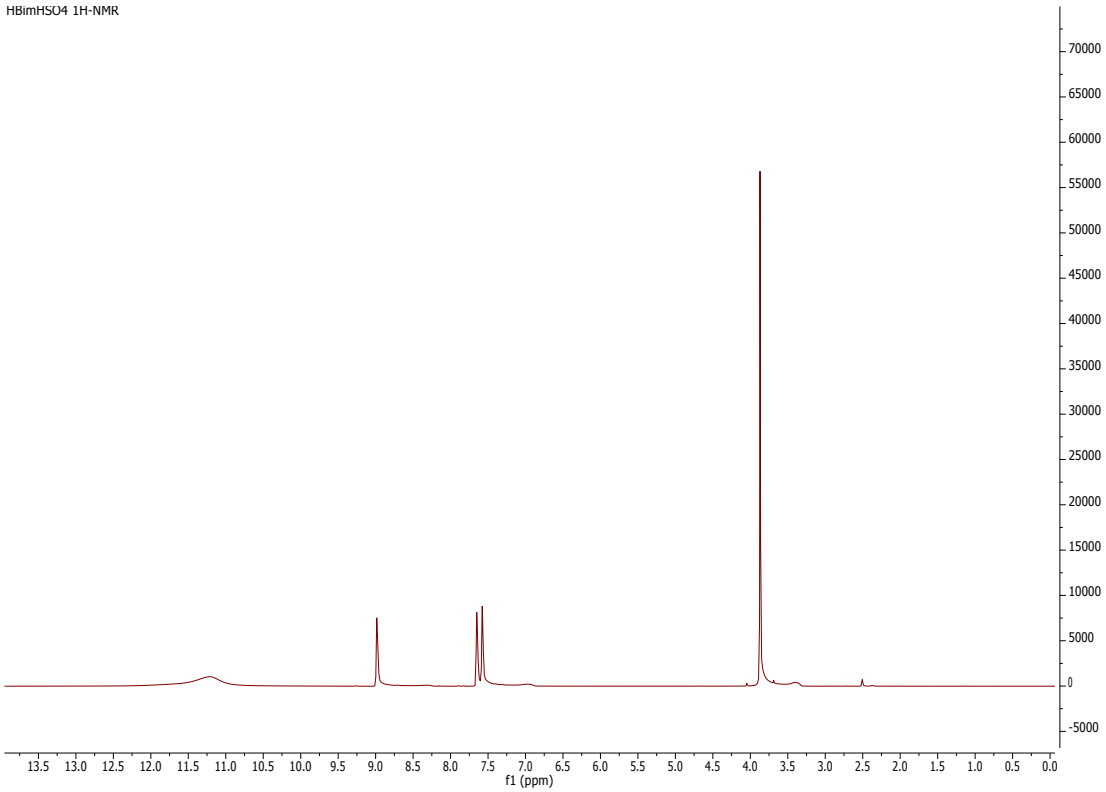
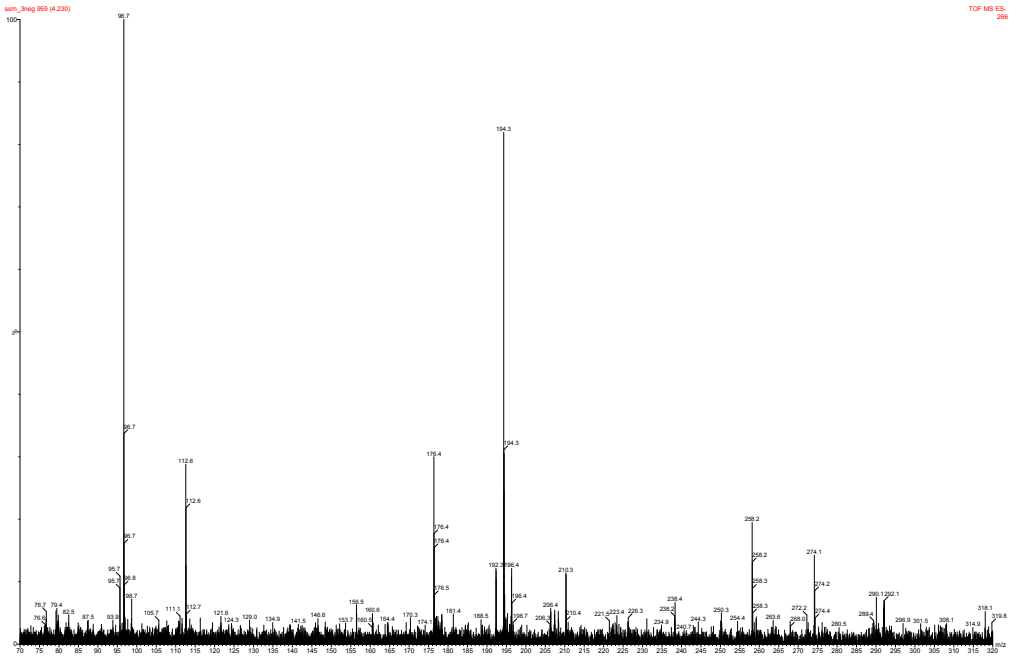


Figure S3 ^{1}H-NMR of IL2



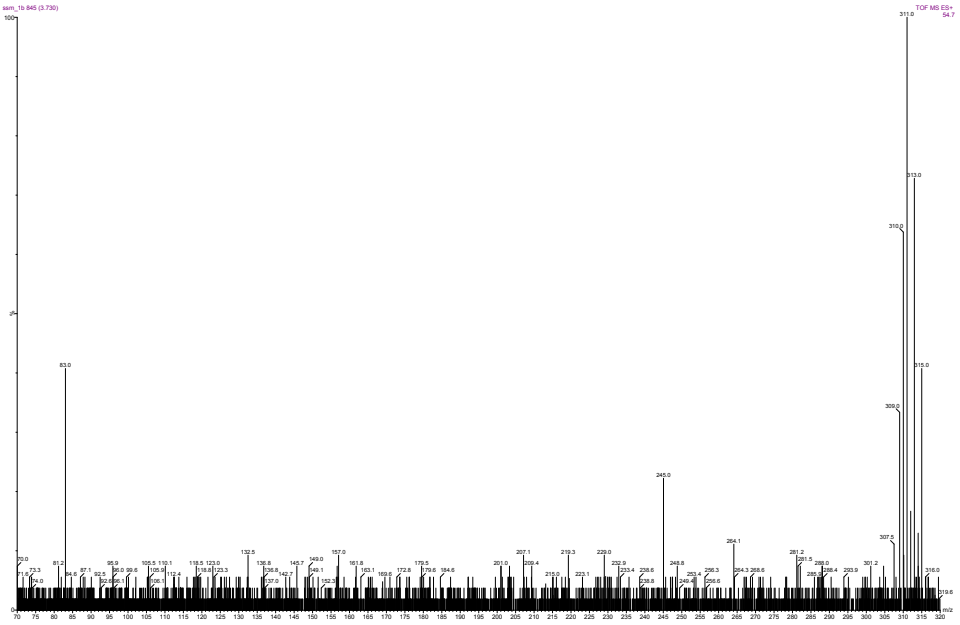


Figure S4 Mass spectra of IL2

2. Simulation results

The following section describes the simulation and reactor design for production of IL1 and IL2. The results are presented for the conventional process and intensified process, respectively.

2.1 The conventional process for IL1

The process configuration is shown in Figure S5 and consists of a single reactor which runs in adiabatic mode. This is because the heat transfer area of a CSTR reactor would be too small to remove the reaction heat and the temperature rise needs to be controlled by a diluting media. In this process water is added to the mixture to an extent that the temperature of the rector is limited to 90^{o}C. Then the pressure is reduced and the medium is heated up and enters a flash drum. The temperature of the flash drum is selected so the concentration of water is reduced from 58.6%wt to 20%wt. The remaining 20% is needed in order to reduce the IL viscosity to a convenient level (~3cP). The separated water needs to be condensed and pumped back for recycle/reuse.

The required power for pumping is calculated based on the parameters in Table S2. The heat duties of coolers/heaters are calculated based on Table S2. The stream data is shown in Table S3. This information will be later applied to make a comparison with the intensified process.

Table S1 Model summary (pumps)

Name	P-1	P-2	P-3	P-4
Electricity [kW]	2.56922	2.64357	4.65179	6.63282
Volumetric flow rate [cum/hr]	4.57766	4.87975	12.7403	21.3423
Calculated discharge pressure [bar]	7	7	7	7

Table S2 Model summary (coolers).

Name	CONDSR	HTX	PROD-CLR
Specified pressure [bar]	-0.3	-0.3	-0.3
Specified temperature [C]	25		25
Specified vapor fraction		0.766	
Calculated heat duty [Gcal/hr]	-13.228	12.1722	-0.888768

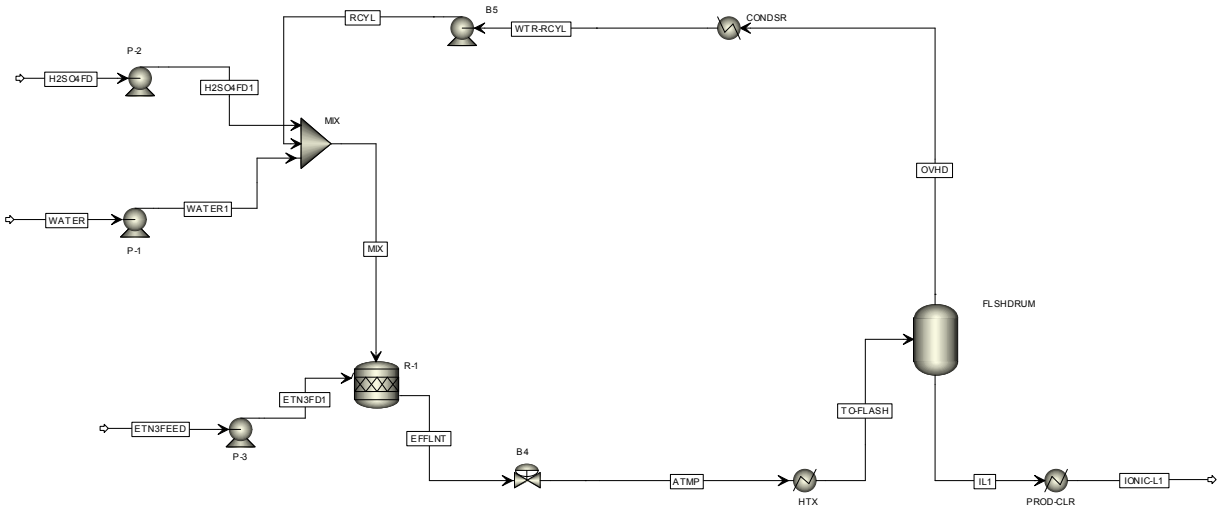


Figure S5 Process flow diagram for the conventional process for IL1 production.

Table S3 Stream table for Figure S5

Steam Tag	ATMP	EFFLNT	ETN3FD1	ETN3FEED	H2SO4FD	H2SO4FD1	IL1	IONIC-L1	MIX	OVHD	RCYL	TO-FLASH	WATER	WATER1	WTR-RCYL
Temperature C	90	90	25.9	25	25	26.2	118.8	25	25.4	118.8	25.3	124.6	25	25.5	25
Pressure bar	2	6.7	7	1	1	7	1.4	1.1	7	1.4	7	1.7	1	7	1.1
Vapor Frac	0	0	0	0	0	0	0	0	0	1	0	0.766	0	0	0
Mole Flow kmol/hr	1521.385	1521.385	91.25	91.25	91.25	91.25	343.868	343.868	1521.385	1177.517	1177.517	1521.385	252.563	252.563	1177.517
Mass Flow kg/hr	43947.81	43947.81	9233.755	9233.755	8949.753	8949.753	22734.51	22734.51	34714.03	21213.29	21213.29	43947.81	4550	4550	21213.293
Mole Flow kmol/hr															
H2SO4	0	0	0	0	91.25	91.25	0	0	91.25	0	0	0	0	0	0
ETN3	0	0	91.25	91.25	0	0	0	0	0	0	0	0	0	0	0
H2O	1430.135	1430.135	0	0	0	0	252.618	252.618	1430.135	1177.517	1177.517	1430.135	252.563	252.563	1177.517
IL1	91.25	91.25	0	0	0	0	91.25	91.25	0	0	0	91.25	0	0	0
Mole Frac															
H2SO4	0	0	0	0	1	1	0	0	0.06	0	0	0	0	0	0
ETN3	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
H2O	0.94	0.94	0	0	0	0	0.735	0.735	0.94	1	1	0.94	1	1	1
IL1	0.06	0.06	0	0	0	0	0.265	0.265	0	0	0	0.06	0	0	0

2.2 The intensified process for IL1

The simplified process configuration is shown in Figure S6 and consists of a series of reactors with interstage coolers. Each reactor operates in an adiabatic mode and is designed based on 100% conversion of sulfuric acid. Sulfuric acid is the limiting reactant and is fed between the stages. The heat of the exothermic reaction results in a temperature rise in the reactor which is a process design decision variable. The extent of interstage cooling is also another decision variable as it affects the temperature of the next reactor. Finally and most importantly, the number of stages is an important design variable and determines the extent of reaction in each stage so the overall reaction will reach completion at the end of the reactor network.

The design specifications applied in this study are shown in Table 1. The IL is solid in the pure state at room temperature. Therefore, the sulfuric acid is diluted with water to maintain a liquid state. The extent of this dilution is adjusted so the ultimate product contains 20 wt % water. The justification for the other specification is to ensure safe operation. For example, the specification of maximum temperature of 90 ^{o}C and minimum pressure of 4 bar will ensure that no evaporation will happen inside the reactor. The analysis shows that avoiding such a limit without using diluting water requires that the extent of the reaction conversion be limited to less than 12.5%, therefore, at least eight reactors are needed. Table S4 reports the stream data. The required power for pumping is reported in Table S5. The heat duties of coolers are reported in Table S6. This information will be applied later for evaluating the operating and capital costs.

The detailed design of reactors was conducted using the results from the simplified flow diagram. In this research, in order to avoid any uncertainty associated with the physical properties of the new ionic liquid product, the heat duties of all reactors are overdesigned up to 100%. The selected material was titanium, to prevent corrosion. The Exchanger Design and Rating software applied built-in optimization in order to minimize the total costs.

The results for the detailed reactor design are shown in Table S7. In addition, Figure S3 shows the diagram of the 8th reactor. The overall bare equipment cost is minimized to only 116800$ and there is no need for extra diluting water and associated costs of separation and recycling.

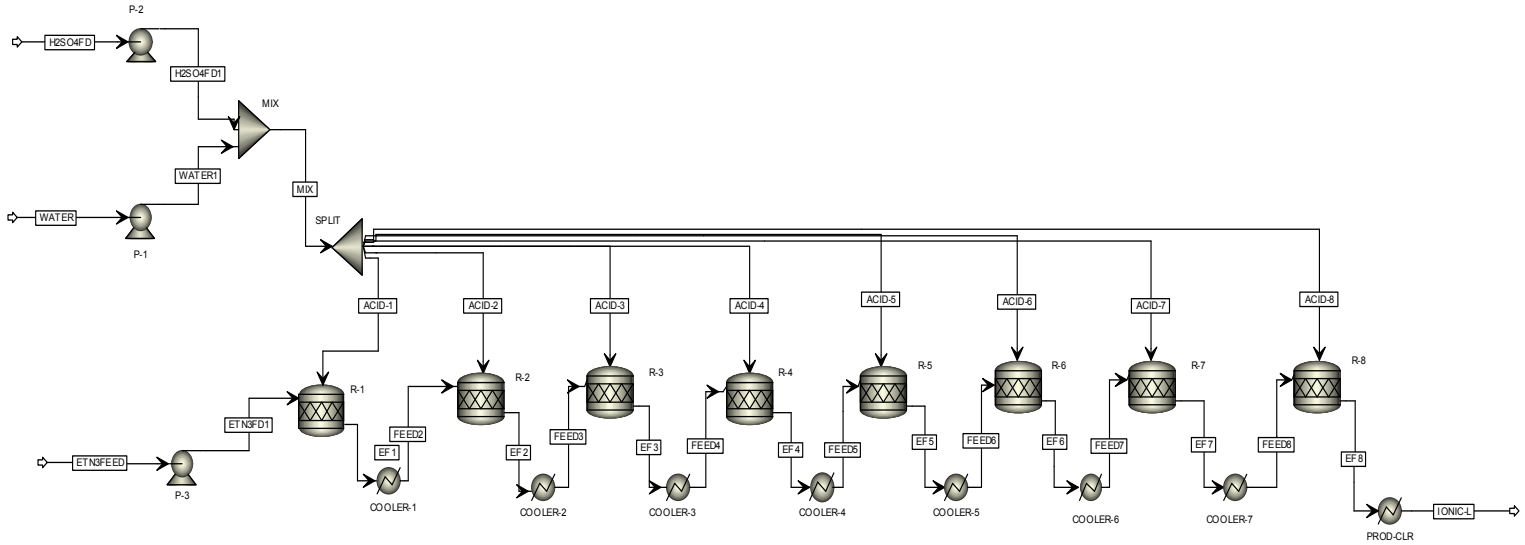


Figure S6 Process flow diagram for the intensified process for IL1 production.

Table S4 Stream table for Figure S6

	ACID-1	ACID-2	ACID-3	ACID-4	ACID-5	ACID-6	ACID-7	ACID-8	EF1	EF2	EF3	EF4	EF5	EF6	EF7	EF8
Temperature C	25.7	25.7	25.7	25.7	25.7	25.7	25.7	25.7	74.9	82.8	79.2	77.1	75.7	74.5	73.6	72.9
Pressure bar	7	7	7	7	7	7	7	7	7	6.7	6.4	6.1	5.8	5.5	5.2	4.9
Vapor Frac	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/hr	42.949	42.949	42.949	42.949	42.949	42.949	42.949	42.949	122.793	154.336	185.879	217.422	248.965	280.508	312.051	343.593
Mass Flow kg/hr	1686.974	1686.974	1686.974	1686.974	1686.974	1686.974	1686.974	1686.974	10920.73	12607.71	14294.68	15981.66	17668.64	19355.61	21042.59	22729.56
Volume Flow cum/hr	1.372	1.372	1.372	1.372	1.372	1.372	1.372	1.372	14.788	16.341	17.881	19.523	21.222	22.957	24.717	26.495
Mole Flow kmol/hr																
H2SO4	11.406	11.406	11.406	11.406	11.406	11.406	11.406	11.406	0	0	0	0	0	0	0	0
ETN3	0	0	0	0	0	0	0	0	79.844	68.438	57.031	45.625	34.219	22.813	11.406	0
H2O	31.543	31.543	31.543	31.543	31.543	31.543	31.543	31.543	31.543	63.086	94.629	126.172	157.715	189.258	220.801	252.343
IL1	0	0	0	0	0	0	0	0	11.406	22.813	34.219	45.625	57.031	68.438	79.844	91.25
Mole Frac																
H2SO4	0.266	0.266	0.266	0.266	0.266	0.266	0.266	0.266	0	0	0	0	0	0	0	0
ETN3	0	0	0	0	0	0	0	0	0.65	0.443	0.307	0.21	0.137	0.081	0.037	0
H2O	0.734	0.734	0.734	0.734	0.734	0.734	0.734	0.734	0.257	0.409	0.509	0.58	0.633	0.675	0.708	0.734
IL1	0	0	0	0	0	0	0	0	0.093	0.148	0.184	0.21	0.229	0.244	0.256	0.266

Table S4 Stream table for Figure S6 (continued)

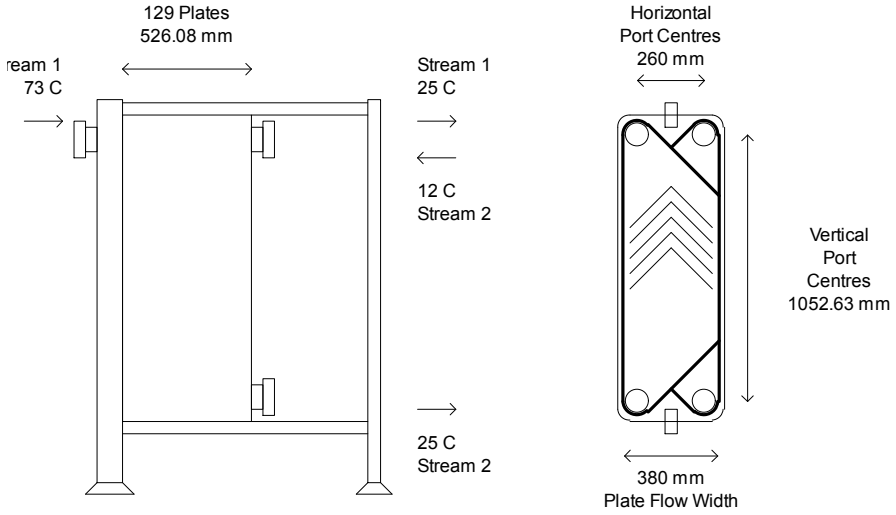
	ETN3FEED	FEED2	FEED3	FEED4	FEED5	FEED6	FEED7	FEED8	H2SO4FD	IONIC-L	MIX	WATER
Temperature C	25	50	50	50	50	50	50	50	25	25	25.7	25
Pressure bar	1	6.7	6.4	6.1	5.8	5.5	5.2	4.9	1	4.6	7	1
Vapor Frac	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/hr	91.25	122.793	154.336	185.879	217.422	248.965	280.508	312.051	91.25	343.593	343.593	252.343
Mass Flow kg/hr	9233.755	10920.73	12607.71	14294.68	15981.66	17668.64	19355.61	21042.59	8949.753	22729.56	13495.79	4546.038
Mole Flow kmol/hr												
H2SO4	0	0	0	0	0	0	0	0	91.25	0	91.25	0
ETN3	91.25	79.844	68.438	57.031	45.625	34.219	22.813	11.406	0	0	0	0
H2O	0	31.543	63.086	94.629	126.172	157.715	189.258	220.801	0	252.343	252.343	252.343
IL1	0	11.406	22.813	34.219	45.625	57.031	68.438	79.844	0	91.25	0	0
Mole Frac												
H2SO4	0	0	0	0	0	0	0	0	1	0	0.266	0
ETN3	1	0.65	0.443	0.307	0.21	0.137	0.081	0.037	0	0	0	0
H2O	0	0.257	0.409	0.509	0.58	0.633	0.675	0.708	0	0.734	0.734	1
IL1	0	0.093	0.148	0.184	0.21	0.229	0.244	0.256	0	0.266	0	0

Table S5 Model summary (pumps)

Name	P-1	P-2	P-3
Electricity [kW]	2.56825	2.64357	4.65179
Volumetric flow rate [cum/hr]	4.57368	4.87975	12.7403
Calculated discharge pressure [bar]	7	7	7

Table S6 Model summary (coolers). Please note that the heat duty of each cooler is equal to the heat generated by the reaction at that stage.

Name	COOLER-1	COOLER-2	COOLER-3	COOLER-4	COOLER-5	COOLER-6	COOLER-7	PROD-CLR
Specified pressure [bar]	-0.3	-0.3	-0.3	-0.3	-0.3	-0.3	-0.3	-0.3
Specified temperature [C]	50	50	50	50	50	50	50	25
Specified vapor fraction								
Calculated heat duty [Gcal/hr]	-0.154792	-0.234397	-0.22839	-0.22583	-0.22321	-0.22012	-0.21671	-0.43641



Actual surface area	51.6 m2	Plate thickness	0.6 mm
Number of passes Stream 1 / 2	2 / 1	Compressed plate pitch	4.11 mm
Effective channels Stream 1 / 2	64 / 64	Area of each plate	.4 m2
Number of exchangers	1	Chevron angle (to horizontal)	45
		Material type	Titanium
		Port diameter	100 mm

Figure S7 The geometric diagram of the final reactor (R-8).

Table S7 The results of the detailed reactor design for IL1 (intensified).

	Heat duty (kw) Overdesign	**Heat duty (kw) Actual**	**Maximum allowable temperature (°C)**	**Exit temperature (°C)**	**Overall heat transfer coefficient**	**Effective Heat transfer area (m^2)**	**Number of plates**	**Material**	**Costs (USD)**
R-1	-360	-180.02314	75	50	2017.5	5.3	29	Titanium	6130
R-2	-540	-272.60389	83	50	1560.7	8.8	35	Titanium	9604
R-3	-530	-265.62234	79	50	1475	8.8	35	Titanium	9604
R-4	-520	-262.64477	77	50	1198.2	9.9	39	Titanium	10678
R-5	-520	-259.58718	76	50	1526.2	8.6	21	Titanium	9300
R-6	-510	-256.00292	75	50	1307.6	9.5	23	Titanium	10194
R-7	-500	-252.03838	74	50	1316.4	9.5	23	Titanium	10194
R-8	-1000	-507.5398	73	25	1033	50.8	129	Titanium	51095
Total									116799

2.3 The conventional process for IL2

The process configuration is shown in Figure S8 and consists of a single reactor which runs in adiabatic mode. The reason is that the heat transfer area of a CSTR reactor would be too small to remove the heat of reaction and the temperature rise needs to be controlled by adding a diluent. In this process water is added to the mixture to an extent that the temperature of the rector is limited to 90^{o}C. Then the pressure is reduced and the medium is heated up and enters a flash drum. The temperature of the flash drum is selected so the concentration of water is reduced from 65%wt to 20%wt. The remaining 20% is needed in order to reduce the IL viscosity to a level (~3cP) convenient for storage and transportation. The separated water needs to be condensed and pumped back for recycle / reuse. The required power for pumping is reported in Table S8. The heat duties of coolers are reported in Table S9. The stream data is shown in Table S10. This information will be later applied to make a comparison with the intensified process.

Table S8 Model summary (pumps).

Name	P-1	P-2	P-3	P-4
Electricity [Watt]	2442.58	2698.08	2911.94	7613.68
Volumetric flow rate [cum/sec]	0.0011463	0.001272	0.00149883	0.00816004
Calculated discharge pressure [N/sqm]	730000	730000	730000	700000

Table S9 Model summary (coolers). Please note that the heat duty of each cooler is equal to the heat generated by the reaction at that stage.

Name	CONDSR	HTX	PROD-CLR
Specified pressure [N/sqm]	-0.3	-30000	-30000
Specified temperature [C]	25	125.85	25
Specified vapor fraction			
Calculated heat duty [kW]	-21284.5	19612.8	-1451.6

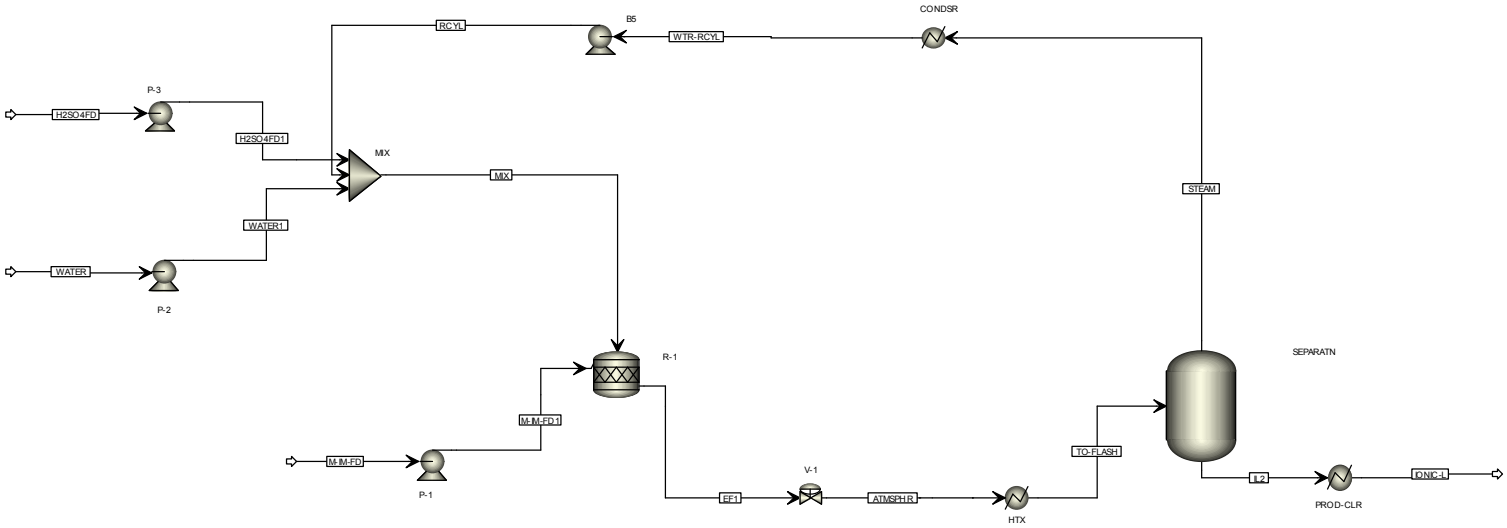


Figure S8 Process flow diagram of the conventional process for IL2 production.

Table S10 Stream table for Figure S8

	ATMSPHR	EFFLNT	H2SO4	H2SO4FD	H2SO4FD1	IL2	IONIC-L	M-IM-FD	M-IM-FD1	MIX	RCYL	STEAM	TO-FLASH	WATER	WATER1	WTR-RCYL
Temperature K	363.1	363.1	343.1	298.1	298.9	399	298.1	298.1	298.7	298.5	298.4	399	399	298.1	298.7	298.1
Pressure N/sqm	200000	700000	500000	100000	730000	170000	140000	100000	730000	700000	700000	170000	170000	100000	730000	169999.7
Vapor Frac	0	0	0	0	0	0	0	0	0	0	0	1	0.821	0	0	0
Mole Flow kmol/sec	0.548	0.548	0.001	0.028	0.028	0.098	0.098	0.028	0.028	0.548	0.45	0.45	0.548	0.07	0.07	0.45
Mass Flow kg/sec	14.425	14.425	0.098	2.749	2.749	6.314	6.314	2.301	2.301	12.124	8.111	8.111	14.425	1.264	1.264	8.111
Mole Flow kmol/sec																
H2SO4	0	0	0.001	0.028	0.028	0	0	0	0	0.028	0	0	0	0	0	0
H2O	0.52	0.52	0	0	0	0.07	0.07	0	0	0.52	0.45	0.45	0.52	0.07	0.07	0.45
M-IMIDAZ	0	0	0	0	0	0	0	0.028	0.028	0	0	0	0	0	0	0
IL2	0.028	0.028	0	0	0	0.028	0.028	0	0	0	0	0	0.028	0	0	0
Mole Frac																
H2SO4	0	0	1	1	1	0	0	0	0	0.051	0	0	0	0	0	0
H2O	0.949	0.949	0	0	0	0.715	0.715	0	0	0.949	1	1	0.949	1	1	1
M-IMIDAZ	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0
IL2	0.051	0.051	0	0	0	0.285	0.285	0	0	0	0	0	0.051	0	0	0

2.4 The intensified process for IL2

The simplified version of the process configuration is shown in Figure S9 and consists of a series of reactors with interstage coolers. Each reactor operates in an adiabatic mode and is designed based on 100% conversion of sulfuric acid which is the limiting reactant and is fed between the stages. The heat of the exothermic reaction results in a temperature rise in the reactor which is a process design decision variable. The extent of interstage cooling is also another decision variable as it affects the temperature of the next reactor. Finally and most importantly, the number of stages is an important design variable and determines the extent of reaction in each stage so the overall reaction will reach completion at the end of the reactor train.

The design specifications applied in this study are shown in Table 1. The IL is a solid in the pure state at room temperature. Therefore, the sulfuric acid is diluted with water in order to maintain a liquid state. The extent of this dilution is selected so the ultimate product contains 20% wt water. The justification for the other specification is to ensure safe operation. For example, the specification of maximum temperature of 95 ^{o}C and minimum pressure of 4 bar will ensure that no evaporation will happen inside the reactor. The analysis shows that avoiding such a limit requires that the extent of the reaction conversion be limited to 9% and eleven reactors are needed. Table S11 reports the stream data. The required power for pumping is reported in Table S12. The heat duties of coolers are reported in Table S13. This information will be applied later for evaluating the operating and capital costs.

The detailed design of reactors was conducted using the results from the simplified simulation. In this research, in order to avoid any uncertainty associated with the physical properties of the new product and materials, the heat duties of all reactors are overdesigned up to 100%. The selected material was titanium. The Exchanger Design and Rating software applied built-in optimization in order to minimize the total costs.

The results for detailed reactor design are shown in Table S14. In addition, Figure S10 shows the diagram of the 11th reactor. The overall equipment costs are minimized to only 110000$ and there is no need for extra diluting water and associated costs of separation and recycling. The costs are based on 2008 and will be later converted to 2012.

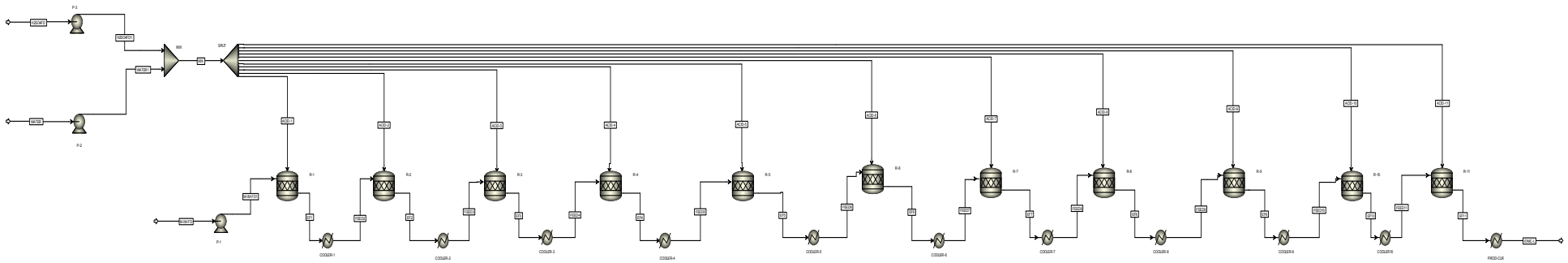


Figure S9 The flow diagram of the intensified process for IL2 production.

Table S11 Stream table for Figure S9.

	ACID-1	ACID-2	ACID-3	ACID-4	ACID-5	ACID-6	ACID-7	ACID-8	ACID-9	ACID-10	ACID-11
Temperature K	298.8	298.8	298.8	298.8	298.8	298.8	298.8	298.8	298.8	298.8	298.8
Pressure atm	7.205	7.205	7.205	7.205	7.205	7.205	7.205	7.205	7.205	7.205	7.205
Vapor Frac	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/hr	35.434	31.891	31.891	31.891	31.891	31.891	31.891	31.891	31.891	31.891	31.891
Mass Flow kg/hr	1446.199	1301.579	1301.579	1301.579	1301.579	1301.579	1301.579	1301.579	1301.579	1301.579	1301.579
Mole Flow kmol/hr											
H2SO4	10.09	9.081	9.081	9.081	9.081	9.081	9.081	9.081	9.081	9.081	9.081
H2O	25.344	22.809	22.809	22.809	22.809	22.809	22.809	22.809	22.809	22.809	22.809
M-IMIDAZ	0	0	0	0	0	0	0	0	0	0	0
IL2	0	0	0	0	0	0	0	0	0	0	0
Mole Frac											
H2SO4	0.285	0.285	0.285	0.285	0.285	0.285	0.285	0.285	0.285	0.285	0.285
H2O	0.715	0.715	0.715	0.715	0.715	0.715	0.715	0.715	0.715	0.715	0.715
M-IMIDAZ	0	0	0	0	0	0	0	0	0	0	0
IL2	0	0	0	0	0	0	0	0	0	0	0

Table S11 Stream table for Figure S9 (Continued).

	EF1	EF2	EF3	EF4	EF5	EF6	EF7	EF8	EF9	EF10	EF11
Temperature K	359.2	365.5	360.1	355.9	352.5	349.8	347.6	345.7	344	342.6	341.4
Pressure atm	7.205	6.908	6.612	6.316	6.02	5.724	5.428	5.132	4.836	4.54	4.244
Vapor Frac	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/hr	126.244	149.053	171.863	194.672	217.482	240.291	263.101	285.91	308.72	331.529	354.339
Mass Flow kg/hr	9730.141	11031.77	12333.39	13635.02	14936.64	16238.27	17539.9	18841.52	20143.15	21444.77	22746.4
Mole Flow kmol/hr											
H2SO4	0	0	0	0	0	0	0	0	0	0	0
H2O	25.344	48.153	70.963	93.772	116.582	139.391	162.201	185.01	207.82	230.629	253.439
M-IMIDAZ	90.81	81.729	72.648	63.567	54.486	45.405	36.324	27.243	18.162	9.081	0
IL2	10.09	19.171	28.252	37.333	46.414	55.495	64.576	73.657	82.738	91.819	100.9
Mole Frac											
H2SO4	0	0	0	0	0	0	0	0	0	0	0
H2O	0.201	0.323	0.413	0.482	0.536	0.58	0.616	0.647	0.673	0.696	0.715
M-IMIDAZ	0.719	0.548	0.423	0.327	0.251	0.189	0.138	0.095	0.059	0.027	0
IL2	0.08	0.129	0.164	0.192	0.213	0.231	0.245	0.258	0.268	0.277	0.285

Table S11 Stream table for Figure S9 (Continued).

	FEED3	FEED4	FEED5	FEED6	FEED7	FEED8	FEED9	FEED10	FEED11	H2SO4FD	IL	IONIC-L	M-IM-FD	MIX	WATER
Temperature K	323.1	323.1	323.1	323.1	323.1	323.1	323.1	323.1	323.1	298.1	343.1	298.1	298.1	298.8	298.1
Pressure atm	6.612	6.316	6.02	5.724	5.428	5.132	4.836	4.54	4.244	0.987	4.935	3.948	0.987	7.205	0.987
Vapor Frac	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/hr	149.053	171.863	194.672	217.482	240.291	263.101	285.91	308.72	331.529	100.9	3.6	354.339	100.9	354.339	253.439
Mass Flow kg/hr	11031.77	12333.39	13635.02	14936.64	16238.27	17539.9	18841.52	20143.15	21444.77	9896.22	648.665	22746.4	8283.89	14461.992	4565.773
Mole Flow kmol/hr															
H2SO4	0	0	0	0	0	0	0	0	0	100.9	0	0	0	100.9	0
H2O	48.153	70.963	93.772	116.582	139.391	162.201	185.01	207.82	230.629	0	0	253.439	0	253.439	253.439
M-IMIDAZ	81.729	72.648	63.567	54.486	45.405	36.324	27.243	18.162	9.081	0	0	0	100.9	0	0
IL2	19.171	28.252	37.333	46.414	55.495	64.576	73.657	82.738	91.819	0	3.6	100.9	0	0	0
Mole Frac															
H2SO4	0	0	0	0	0	0	0	0	0	1	0	0	0	0.285	0
H2O	0.323	0.413	0.482	0.536	0.58	0.616	0.647	0.673	0.696	0	0	0.715	0	0.715	1
M-IMIDAZ	0.548	0.423	0.327	0.251	0.189	0.138	0.095	0.059	0.027	0	0	0	1	0	0
IL2	0.129	0.164	0.192	0.213	0.231	0.245	0.258	0.268	0.277	0	1	0.285	0	0	0

Table S12 Model summary (pumps).

Name	P-1	P-2	P-3
Electricity [Watt]	2442.58	2701.75	2911.94
Volumetric flow rate [cum/sec]	0.001146	0.001276	0.001499
Calculated discharge pressure [N/sqm]	730000	730000	730000

Table S13 Model summary (coolers). Please note that the heat duty of each cooler is equal to the heat generated by reaction at that stage.

Name	**COOLER-1**	**COOLER-2**	**COOLER-3**	**COOLER-4**	**COOLER-5**	**COOLER-6**	**COOLER-7**	**COOLER-8**	**COOLER-9**	**COOLER10**	**CWCAL**	**HEATER**	**PROD-CLR**
Calculated pressure [N/sqm]	700000	670000	640000	610000	580000	550000	520000	490000	460000	430000	670000	100000	400000
Calculated temperature [K]	323.15	323.15	323.15	323.15	323.15	323.15	323.15	323.15	323.15	323.15	298.15	284.2	298.15
Calculated vapor fraction	0	0	0	0	0	0	0	0	0	0	0	0	0
Calculated heat duty [kW]	-186.36	-258.263	-258.279	-258.292	-258.302	-258.311	-258.319	-258.326	-258.331	-258.337	150	0.29	-603.929

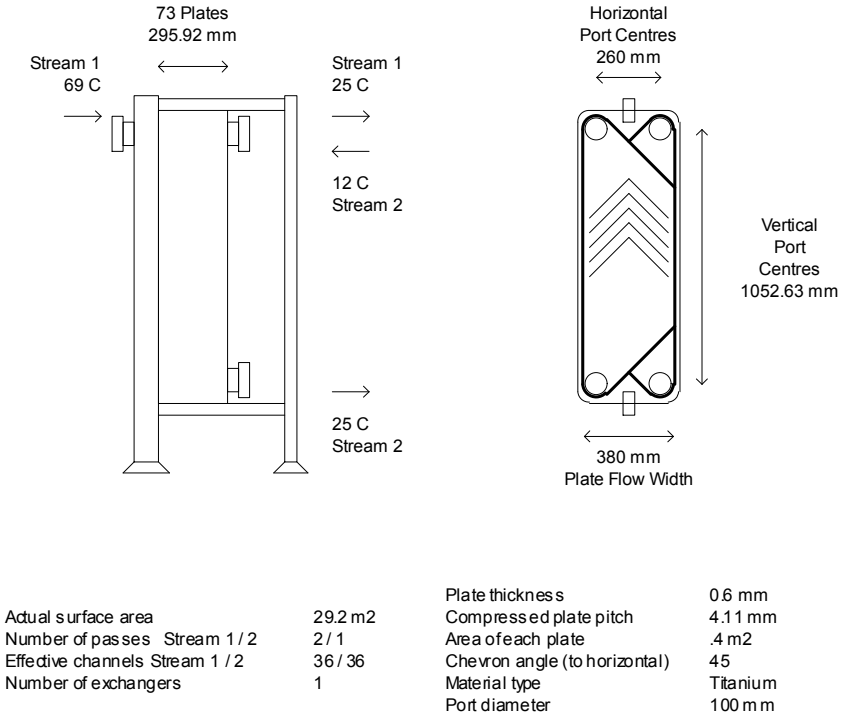


Figure S10 The geometric diagram of the 11th reactor.

Table S14. The results of the detailed reactor design for IL2 (intensified).

	Heat duty (kw) Overdesign	**Heat duty (kw) Actual**	**Maximum allowable temperature (oC)**	**Exit temperature (oC)**	**Overall heat transfer coefficient**	**Effective Heat transfer area (m2)**	**Number of plates**	**Material**	**Costs (USD)**
R-1	-370	-186.4	86	50	1072.6	7.1	49	Titanium	8074
R-2	-520	-258.3	93	50	1021.1	9.9	39	Titanium	10678
R-3	-520	-258.3	87	50	1477.6	7.8	31	Titanium	8529
R-4	-520	-258.3	83	50	1695.8	7.8	31	Titanium	8529
R-5	-520	-258.3	80	50	1485.7	7.7	19	Titanium	8407
R-6	-520	-258.3	77	50	1710.3	7.2	29	Titanium	7991
R-7	-520	-258.4	75	50	2017.5	6.1	25	Titanium	6916
R-8	-520	-258.4	73	50	2127.8	6.1	25	Titanium	6916
R-9	-520	-258.4	71	50	2132.7	6.8	17	Titanium	7512
R-10	-520	-258.4	70	50	2212.4	6.8	17	Titanium	7512
R-11	-1200	-603.6	69	25	2051.7	28.4	73	Titanium	28926
Total									109990

3. Economic assessment

The purchase cost for a given component reflects a baseline equipment size. As changes are made to the process, the plant capacity may be different from what was originally designed, which will accordingly affect the equipment purchased cost. A common guideline for extrapolation of cost estimation to a different volume is the six-tenths rule:

$$New\ Cost = (Base\ Cost)(\frac{New\ Size}{Base\ Size})^{0.6}$$

So the new equipment purchased cost can be easily estimated as changes are made to the plant capacity.

C_{OL} is determined based on data obtained from five chemical companies and correlated by W.A. Alkayatet al.[9] According to this method, the operating labour requirement for chemical processing plants is given by

$$N_{OL} = (6.29 + 31.7\ P^2 + 0.23N_{np})^{0.5}$$

where N_{OL} is the number of operators per shift, P is the number of processing steps involving the handling of particulate solids—for example, transportation and distribution, particulate size control, and particulate removal. N_{np} is the number of non-particulate processing steps and includes compression, heating and cooling, mixing and reaction. In this IL preparation process, there is no solid participating in the system. For instance, in the intensified process for ILs production, $N_{np}$is determined as 8 (8 reactors). So N_{OL} of this system is calculated as 2.85.

A single operator is assumed to work on average 49 weeks a year (3 weeks' time off for vacation and sick leave), with five 8-hour shifts a week. This amounts to (49 weeks/year × 5 shifts/week) 245 shifts per operator per year. A chemical plant normally operates 24 hours/day. This requires (330 days/year × 3 shifts/day) 990 operating shifts per year. The number of operators needed to provide this number of shifts is [(990 shifts/yr)/(245 shifts/operator/yr)] or approximately 4 operators. Four operators are hired for each operator needed in the plant at any time. This provides the needed operating labour but does not include any support or supervisory staff. The number of operators required per shift is 2.85. So 11.4 (4×2.85) operators are needed totally (rounding up to the nearest integer yields 12 operators).

From the US Department of Labour (http://www.bls.gov/oes/current/oes_nat.htm#51-0000), it is known that the operators' annual mean wages are generally around $50,000 in 2012. Herein, we adopt $50,000 for the labour cost calculation.